SENSITIVITY ANALYSIS AND COMPUTATION FOR PARTIAL DIFFERENTIAL EQUATIONS

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Principal Investigator:

Lisa G. Davis

Montana State University
Department of Mathematical Sciences
PO Box 172400
Bozeman, MT 59717–2400
Voice: 406-994-5347, Fax: 406-994-1789
davis@math.montana.edu

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The development of practical numerical methods for simulation of partial differential equations leads to problems of convergence, accuracy and efficiency. Verification of a computational algorithm consists in part of establishing a convergence theory for the discretized equations. It is well known that the long time behavior of a system may not be captured even by ``convergent'' approximating methods and additional requirements must be placed on the scheme to ensure the discretized equations capture the correct asymptotic behavior. Even on finite intervals, there are always uncertainties in the problem data that can be a source of difficulty for accurate simulation of nonlinear problems. These uncertainties lead to uncertainty in the computed results and should be considered as part of the verification step. This research gives preliminary results showing how sensitivity analysis can be used to provide a practical precursor to dynamic transitions and quantify numerical uncertainty in simulations of nonlinear parabolic partial differential equations.

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Abstract

The development of practical numerical methods for simulation of partial differential equations leads to questions of convergence, accuracy (in time and space) and efficiency. Verification of a computational algorithm includes the process of establishing a convergence theory for the discretized equations. It is well known that the long time behavior of a system may not be captured even by "convergent" approximating methods and additional requirements must be placed on the scheme to ensure the discretized equations capture the correct asymptotic behavior. Even on finite intervals, there are always uncertainties in the problem data that can be a source of difficulty for accurate simulation of nonlinear problems. These uncertainties lead to uncertainty in the computed results and should be considered as part of the verification step. This research gives preliminary results showing how sensitivity analysis can be used to provide a practical precursor to dynamic transitions and quantify numerical uncertainty in simulations of nonlinear parabolic partial differential equations.

Contents

1 Summary and Objectives

Research Objective: It is well known that the long time behavior of a nonlinear dynamical system may not be captured even by convergent approximating methods and additional requirements must be placed on the scheme to ensure the discretized equations capture the correct asymptotic behavior. This issue is particularly important when one is forced to use numerical methods to evaluate the asymptotic behavior of a closed-loop control system when the mathematical model is defined by a nonlinear partial differential equation (PDE). In addition, using feedback to eliminate or delay transition in fluid flows often requires some type of mechanism to predict that a transition is about to occur. The recent papers [3], [4], [5], [21] and [22] provide considerable evidence that, for certain nonlinear systems that occur in fluid flows, sensitivity analysis can be used to indicate a transition is about to occur. In [4] and [5] it was shown that this information can be used to determine when to turn on a controller to prevent transition. This report illustrates that similar sensitivity tools can also be used to provide insight into the asymptotic behavior of the closed-loop system. In particular, it is shown that time varying sensitivities can be used to determine when a numerical simulation is correctly predicting the longtime behavior of the response. In the cases considered here, the trigger of a transition can be a known parameter (wall roughness, etc.) or an un-modeled uncertainty in the problem data. This includes uncertainty in parameters, initial data, boundary conditions and forcing terms. These uncertainties in the problem data lead to uncertainty in the computed results and should be considered as part of a verification step. In addition, although we do not address this issue here, it has recently been observed that finite precision arithmetic and sensitivity to parameter uncertainty can

lead to orders of magnitude errors in simulations of simple nonlinear convection-diffusion equations (see [1] and [3]). The focus of this report is on a nonlinear reaction-diffusion equations to illustrate the problem and method. However, we first present a simple ODE example to illustrate some of the basic ideas.

Collaborators: Dr. John A. Burns of the Interdisciplinary Center for Applied Mathematics and the Department of Mathematics at Virginia Tech served as the main collaborator for this work. The results in this report, along with the results that are currently in preparation in a more extensive manuscript, were the result of an intense two week period of collaboration between the PI and Dr. Burns and a considerable amount of subsequent communication. In addition, the ideas for the first example came from the thesis problem and subsequent work of Dr. John R. Singler of the Mechanical Engineering Department at Oregon State University. His results and observations for the simple control problem example were quite useful and much appreciated.

2   Results of Funding

The following sections illustrate the key ideas of how sensitivity analysis can be used to predict the onset of *transition* in various numerical simulations. The first example is that of a simple closed-loop control system, and the second section contains an example of a classical nonlinear parabolic partial differential equation. In each case, by choosing to examine the sensitivity of the state variable with respect to a certain parameter, we are able to produce numerical sensitivity simulations which serve as an indicator that a transition is about to take place in the behavior of the original state variable.

2.1   A Finite Dimensional Example

We consider a 3D system that is typical of those found in the papers [4], [5], [20], [21], [25], [26] and [27]. However, we focus on the role that small constant disturbances play in transition and illustrate how sensitivity information can be used to predict the transition in these cases. The system is governed by three ordinary differential equations and has the form

$$\dot{x}(t) = A(R)x(t) + \|x(t)\| \, Sx(t) + Bu(t) + Dq, \quad x(0) = x_0, \tag{2.1}$$

where $A(R) = [\frac{1}{R}A_0 + R]$, $A_0 < 0$ is diagonal and $S = -S^*$ is skew-adjoint. In particular, this three dimensional system is defined by

$$A(R) = \begin{bmatrix} -\alpha/R & 1 & 0 \\ 0 & -\beta/R & 1 \\ 0 & 0 & -\gamma/R \end{bmatrix}, \tag{2.2}$$

$$S = \begin{bmatrix} 0 & -b_1 & -b_2 \\ b_1 & 0 & b_3 \\ b_2 & -b_3 & 0 \end{bmatrix} \tag{2.3}$$

and

$$B = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, D = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \tag{2.4}$$

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where all constants are positive. Here, q is considered a "small" constant (un-modeled) disturbance. For the runs here we set $\alpha = 0.5$, $\beta = 0.75$, $\gamma = 1.0$, $b_1 = 1.0$, $b_2 = 0.5$ and $b_3 = 0.25$. The linear operator $A(R)$ is stable for all $R > 0$ and for the no disturbance case (i.e. when $q = 0$) the dynamical system is also dissipative. In particular, the nonlinear system (2.2)-(2.4) has a compact global attractor. The problem is sensitive to the parameter q and this sensitivity plays an important role in the transition process.

Let

$$s(t) \triangleq \frac{\partial x(t, q)}{\partial q}\Big|_{q=0} = \frac{\partial x(t, 0)}{\partial q} \tag{2.5}$$

denote the sensitivity of the solution $x(t) = x(t, q)$ at $q = 0$. It follows that the sensitivity $s(t)$ satisfies the linear differential equation

$$\dot{s}(t) = A(R)s(t) + \boldsymbol{F}(x(t))s(t) + D, \quad s(0) = 0, \tag{2.6}$$

where

$$\boldsymbol{F}(x) = \begin{cases} \|x\| \, S + Sxx^T / \|x\|, & x \neq 0 \\ 0, & x = 0 \end{cases}.$$

Consider the case where $x_0 = [9, 9, 9]^T \times 10^{-6}$ and $q = 5 \times 10^{-8}$. Figure 1 below contains the plots of the norms of solution $x(t, q)$ and the sensitivity $s(t)$ (top plot) for this system. Observe that the solution does not "transition" to the (chaotic) attractor until $t = 175 seconds$. However, at $t = 50 seconds$ the sensitivity $s(t)$ satisfies $\|s\| > 10^3$. The vertical red line at $t = 50 seconds$ indicates that the sensitivity information provides a precursor to the upcoming transition long before the transition is observable in the state. This precursor was used by Singler to determine when to switch on a capturing feedback controller which is then able to prevent the transition (see [20]).

In the next section we use a similar technique to investigate the numerical simulation of the longtime behavior of a nonlinear parabolic PDE. However, in the PDE case the "sensitive" parameter is in the boundary condition which is typical in parabolic diffusion-convection-reaction equations (see [1], [3], [4], [5], [13], [20] and [21]).

2.2 The Chaffee-Infante Equation

We consider a particular reaction-diffusion equation first studied by Chaffee and Infante in [9] and [10]. This model is a well understood dissipative dynamical system with a global attractor consisting of a finite number of fixed points and the corresponding unstable manifolds (see pages 301 - 306 in [18] for details). In particular, we focus on the partial differential equation

$$z_t(t, x) = z_{xx}(t, x) + \lambda(z(t, x) - [z(t, x)]^2), \quad 0 < x < \pi, \quad t > 0 \tag{2.7}$$

with initial condition

$$z(0, x) = \phi(x), \tag{2.8}$$

and Dirichlét boundary conditions

$$z(t, 0) = 0 = z(t, \pi). \tag{2.9}$$

Here $\lambda > 1$, and in this setting it may be helpful to think of (2.7)-(2.9) as a closed-loop system that we wish to simulate. It is sufficient to consider the case where $\lambda = 4.1$ so that the following result holds (see page 303 in [18]).
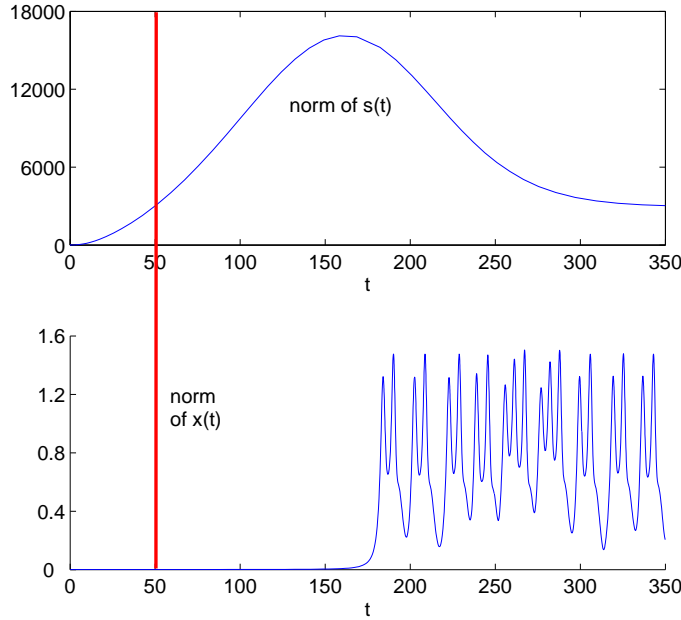
Figure 1: Norm of $x(t)$ and $s(t)$

Theorem 2.1. *If $\lambda = 4.1$, then the system (2.7)-(2.9) has five fixed points $\phi_0(\cdot) \equiv 0$, $\phi_1^+(\cdot)$, $\phi_1^-(\cdot)$, $\phi_2^+(\cdot)$ and $\phi_2^-(\cdot)$ in $L^2(0, \pi)$. The fixed points $\phi_0(\cdot) \equiv 0$, $\phi_2^+(\cdot)$ and $\phi_2^-(\cdot)$ are unstable and the attractor consists of the unstable manifolds for these fixed points along with the stable fixed points $\phi_1^+(\cdot)$ and $\phi_1^-(\cdot)$.*

Figure 2 is a schematic of the global attractor. However, for certain initial conditions trajectories are pushed rapidly towards the unstable zero fixed point before "transitioning" to one of the stable fixed points $\phi_1^+(\cdot)$ or $\phi_1^-(\cdot)$. This is similar to the previous ODE example except for the fact that this system is not chaotic. However, if one uses standard simulation schemes to investigate the dynamic behavior of this system it is easy to obtain misleading results.

Consider the case where the initial function is given by $\phi(x) = 1.5 \sin(3x)$. Using the Matlab^{TM} routine `pdepe` to simulate (2.7)-(2.9) on the interval $0 < t < 8$, yields the solution shown in Figure 3.

It appears that by $t = 2$ the solution has "converged" to the zero steady state solution. However, since the theorem above tells us that this fixed point is unstable we know that this is unlikely. Indeed, if one continues to run the simulation to $t = 16$ we observe that the solution actually "transitions" to the stable fixed point $\phi_1^-(\cdot)$. This is shown in Figure 4 below. This is also clearly demonstrated in Figure 5 and Figure 6 which contain the plots of the L^2 norms of the solution on the intervals $[0, 8]$ and $[0, 16]$, respectively.

In more complex problems one does not always have the type of qualitative information that is conveniently available for the Chaffee-Infante equation. As illustrated by this example, it is not always clear when a particular numerical solution is producing the proper asymptotic results. Even if the algorithm does **eventually** capture the correct limiting behavior, it is not obvious how long one must run the simulation to see this result. There-
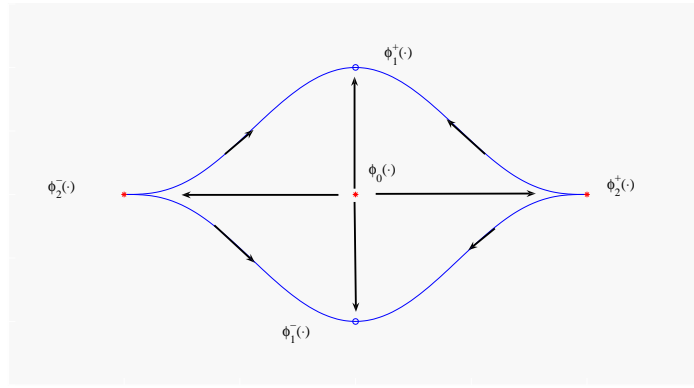
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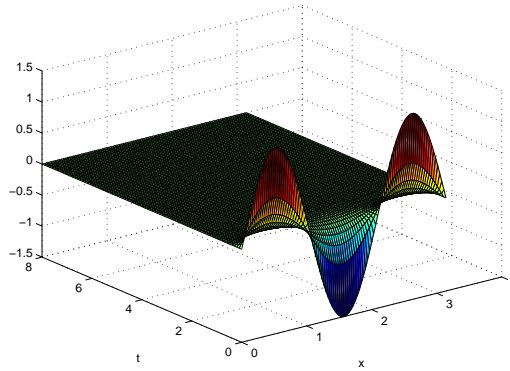Figure 2: Global Attractor for the Chaffee-Infante Equation

Figure 3: $z(t, x)$ on $0 < t < 8$

fore, it is important to devise numerical methods that can help predict when a simulation has "converged" to the correct asymptotic behavior. Equally important is the ability of an algorithm to generate and evaluate secondary information that might indicate when it is **unlikely** that an algorithm has "converged" to the correct asymptotic behavior. Although this is a difficult problem for general systems, in certain cases sensitivity analysis can be helpful in dealing with this issue.

2.3   Boundary Sensitivity for the Chaffee-Infante Equation

Here we consider the sensitivity of the Chaffee-Infante equation with respect to the boundary condition. In particular, we replace the boundary condition (2.9) with the non-homogenous Dirichlét boundary condition

$$z(t, 0) = q = z(t, \pi), \tag{2.10}$$

where q is a "small" number. It can be shown that the Chaffee-Infante equation is highly sensitive to changes in the boundary conditions and this allows us to consider the sensitivity
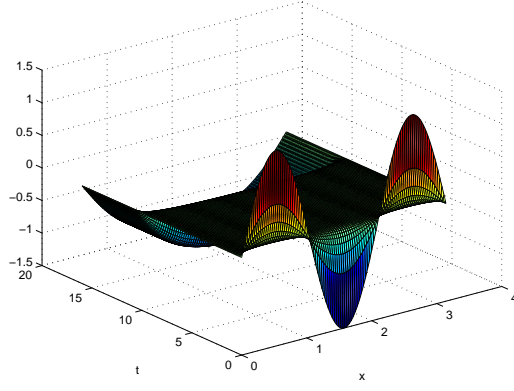
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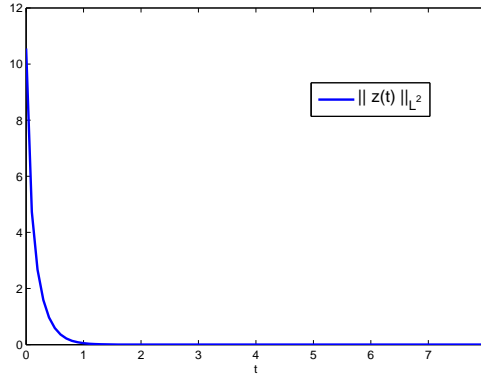Figure 4: $z(t, x)$ on $0 < t < 16$

Figure 5: L^2 norm of $z(t, \cdot)$ on $0 < t < 8$

variable

$$s(t,x) \triangleq \frac{\partial z(t,x,q)}{\partial q}\Big|_{q=0} = \frac{\partial z(t,x,0)}{\partial q}$$

to analyze this sensitivity near $q = 0$. The sensitivity $s(t, x)$ satisfies the linear boundary value problem

$$s_t(t,x) = s_{xx}(t,x) + \lambda(s(t,x) - 2[z(t,x)]s(t,x)), \quad 0 < x < \pi, \quad t > 0, \tag{2.11}$$

with initial condition

$$s(0, x) = 0, \quad 0 < x < \pi \tag{2.12}$$

and boundary conditions

$$s(t, 0) = s(t, \pi) = 1, \quad t > 0. \tag{2.13}$$

This sensitivity provides considerable insight into the long-term behavior of the solution to the Chaffee-Infante equation. First note that if the solution $z(t, x) \to \hat{\phi}(x)$ and $\hat{\phi}(x)$ is a stable equilibrium state, then one would expect that the sensitivity $s(t, x)$ would approach
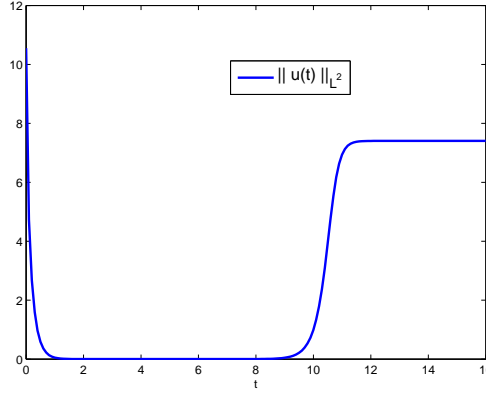
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Figure 6: L^2 norm of $z(t, \cdot)$ on $0 < t < 16$

a steady state $\hat{s}(x)$ satisfying

$$0 = s''(x) + \lambda(s(x) - 2[\hat{\phi}(x)]s(x)), \quad 0 < x < \pi,$$

with boundary conditions

$$s(0) = s(\pi) = 1.$$

In particular, one would have $\lim\limits_{t \to +\infty} \|s(t, \cdot)\|_{L^2} \to \|\hat{s}(x)\|_{L^2} \to c$ where c is a constant.

This is illustrated in Figure 7 and Figure 8 below. Observe that even though the solution $z(t, x)$ appears to have "converged" to the fixed point $\phi_0(x) = 0$ by $t = 2$, and seemingly remains at zero for $2 < t < 8$ (recall the qualitative information in Figure 3 and Figure 5), the sensitivity $s(t, x)$ is growing at an exponential rate on the entire interval $[0, 8]$ as shown in Figure 7, Figure 8 and is best observable in Figure 9. Moreover, when the solution transitions to the stable fixed point $\phi_1^-(\cdot)$ at $t \approx 9$ the sensitivity is maximized and then converges to a (small) steady state as expected. If one compares Figure 8 with Figure 6 above, then it is clear that this sensitivity provides insight into the transition.
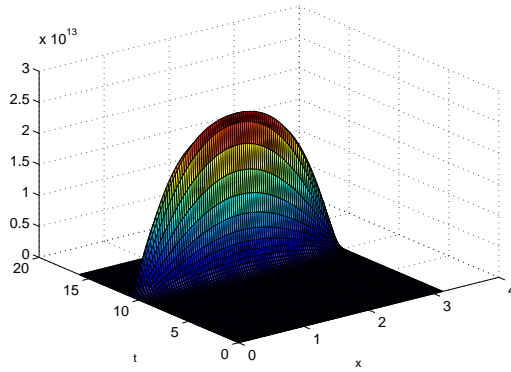

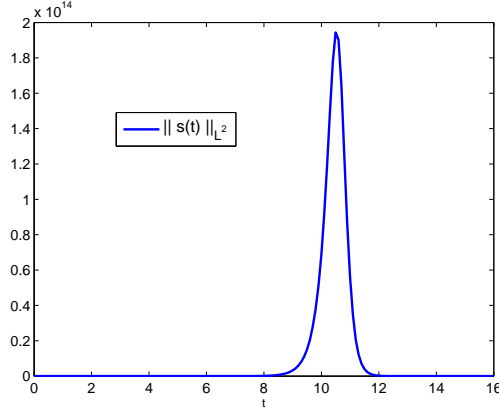Figure 7: $s(t, x)$ on $0 < t < 16$

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Figure 8: L^2 norm of $s(t, \cdot)$ on $0 < t < 16$

The most important observation about the numerical results here is that even on the "short" time interval $0 < t < 8$, when the numerical solution $z(t, x)$ appears to have stabilized at zero, the sensitivity indicates otherwise. In particular, in Figure 9 below we see the exponential growth of $s(t, x)$ on $[0, 8]$ and at $t \approx 7$ the norm of the sensitivity is of the order 10^9. Thus, even on the short time interval $[0, 8]$ the sensitivity provides a clear indication that the solution $z(t, x)$ has not stabilized at a fixed point and that it is **unlikely** that the numerical simulation is "converged". As previously noted, this insight can be used to turn on feedback controllers to prevent transition. Perhaps even more importantly, sensitivity analysis of this type can be used to help evaluate numerical simulations in problems where little is known about the actual asymptotic behavior of the system.
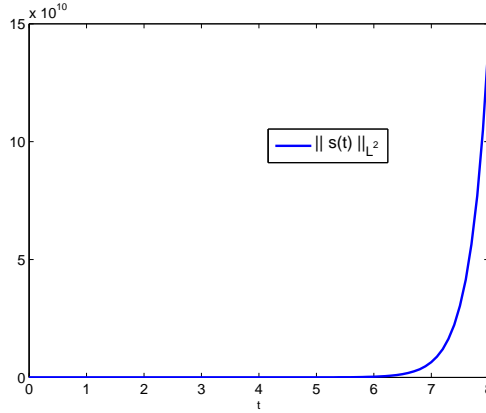

Figure 9: L^2 norm of $s(t, \cdot)$ on $0 < t < 8$

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3 Conclusions and Future Work

In this short report we presented two examples to illustrate how time varying sensitivity analysis can be used for control and to provide insight into the validation of numerical simulations in nonlinear systems. These ideas have also been applied to a wide variety of reaction-convection-diffusion systems, and a complete paper will appear in the future. We note that many convection-diffusion problems, such as Burgers' equation, show extreme sensitivity to boundary perturbations, and sensitivity analysis for these systems has provided amazing insight into the asymptotic behavior of numerical solutions (see [1], [2], [3], [5], [6], [7], [8], [12], [13], [14], [15], [11], [16], [17], [20], [21] and [22]). Problems of this type are infinitely sensitive to small parameter changes and can have a dramatic impact on the convergence of optimal control and design algorithms.

We note that although the numerical results here provide considerable evidence that time varying sensitivities can play an important role in control design and analysis, considerable work needs to be done to place these ideas on a mathematically rigorous foundation. We have some theoretical results for parabolic dissipative systems similar to the Chaffee-Infante equations. However, much work remains to be done. Finally, it is clear that in order to implement some of these ideas, one needs to have some indication of which parameters (modeled or un-modeled) are important to use in the sensitivity analysis. We are currently looking into using Fisher information theory as a mechanism to identify these crucial parameters.

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